Maria Emelianenko

masha@cmu.edu

# List of Publications

http://www.math.cmu.edu/~masha

## 1 Published or submitted

1. Q. Du, M. Emelianenko *"Uniform convergence of a nonlinear energy-based multilevel quantization scheme via centroidal Voronoi tessellations"*, under revision for SIAM J. Numer. Anal., 2006

   Abstract. A popular vector quantization scheme can be constructed by the Centroidal Voronoi tessellations (CVTs) which also have many other applications in diverse areas of science and engineering. The development of efficient algorithms for their construction is a key to the successful applications of CVTs in practice. This paper studies the details of a new optimization based multilevel algorithm for the numerical computation of the CVTs. The rigorous proof of its uniform convergence in one space dimension and the results of computational simulations are provided. They substantiate recent claims on the significant speedup demonstrated by the new scheme in comparison with traditional methods.

2. Q. Du, M. Emelianenko and L. Ju *"Convergence properties of the Lloyd algorithm for computing the centroidal Voronoi tessellations"*, SIAM J. Numer. Anal., 44, Issue 1 (2006), 102-119

   Abstract. Centroidal Voronoi tessellations (CVTs) are Voronoi tessellations of a bounded geometric domain such that the generating points of the tessellations are also the centroids (mass centers) of the corresponding Voronoi regions with respect to a given density function. Centroidal Voronoi Tessellations may also be defined in more abstract and more general settings. Due to the natural optimization properties enjoyed by CVTs, they have many applications in diverse fields. For a given domain, the Lloyd algorithm is one of the most popular iterative schemes for computing the CVTs but its theoretical analysis is far from complete. In this paper, some new analytical results on the local and global convergence of the Lloyd algorithm are presented. These results are derived through careful utilization of the optimization properties shared by CVTs. Numerical experiments are also provided to substantiate the theoretical analysis.

3. M. Emelianenko, Z.-K. Liu and Q. Du *"A New Algorithm for the Automation of Phase Diagram Calculation"*, Comp. Mater. Sci., 35, issue 1 (2006), 61-74 (In ScienceDirect Top 25 Hottest Articles)

   Abstract. We propose a new algorithm for minimizing the Gibbs energy functional and constructing phase diagrams through utilizing geometric properties of the energy surfaces together with effective sampling techniques to improve on the starting points for the minimization. The new method possesses advantages over existing methods in terms of speed and computational complexity and can be used to automate the calculation of phase equilibria in complex systems. Numerical results for binary and ternary systems are presented. Generalizations to higher dimensions are discussed.

4. Q. Du, M. Emelianenko *"Acceleration schemes for computing the centroidal Voronoi tessellations"*, Numer. Linear Algebra Appl.,13, Issue 2-3 (Special Issue on Multigrid Methods) (2006), 173-192

   Abstract. Centroidal Voronoi tessellations have diverse applications in many areas of science and engineering. The development of efficient algorithms for their construction is a key to their success in practice. In this paper, we study some new algorithms for the numerical computation of the centroidal Voronoi tessellations, including the Lloyd-Newton iteration and the optimization based multilevel method. Both theoretical analysis and computational simulations are conducted. Rig-

orous convergence results are presented and significant speedup in computation is demonstrated through the comparison with traditional methods.

5. Q. Du, M. Emelianenko, H.-C. Lee and X. Wang *"Ideal point distributions, best mode selections and optimal spatial partitions via centroidal Voronoi tessellations"*, in proceedings of the 2nd International Symposium on Voronoi Diagrams in Sciences and Engineering (refereed), Seoul, Korea, Oct 2005 (VD2005), pp. 325-333, 2005

Abstract. There are many new applications of the centroidal Voronoi tessellations that have come to life in recent years, along with more mathematical understandings and new algorithmic advances in their efficient computation. Some examples are presented in this paper as an illustration with an emphasis on the construction of ideal point distributions, best mode selections and optimal spatial partitions.

6. Q. Du, M. Emelianenko *"Uniform convergence of a multilevel energy-based quantization scheme"*, to appear in Lect. Notes Comput. Sci. Eng., proceedings of the DD16 conference, Courant Inst., New York, 2005

Abstract. Quantization has diverse applications in many areas of science and engineering. We propose a new multigrid quantization scheme in a nonlinear energy-based optimization setting. The problem of constructing an optimal vector quantizer based on the Centroidal Voronoi Tesselation is nonlinear in nature and hence cannot in general be analyzed using standard linear multigrid approach. We try to overcome this difficulty by essentially relying on the energy minimization. Since the energy functional is in general non-convex, a dynamic nonlinear preconditioner is proposed to relate our problem to a sequence of convex optimization problems. In the case of the one-dimensional problem, we have shown that for a large class of density functions, the nonlinear multigrid algorithm enjoys uniform convergence properties independent of $k$, the problem size, thus a significant speedup comparing to the traditional Lloyd-Max iteration is achieved.

7. M. Yacoubi, M. Emelianenko, N. Gautam) *"Pricing in next generation network queuing model to guarantee QoS"*, Perform. Evaluation, **5**, issue 1 (2003), 59-84 (In Top 10 downloads from Performance Evaluation website in 2003)

Abstract. We consider the scenario where users access Next Generation Networks via Network Access Providers (NAP). We assume that users belong to $N$ different classes and the bandwidth received by each class is determined by a user share differentiation (USD) scheme. According to USD, each class is guaranteed a minimum bandwidth and all users accepted into the NAP are allocated the minimum bandwidth corresponding to their class and any remaining bandwidth is shared according to the ratio of the minimum bandwidths of each class. We develop a queueing-based model and solve an optimization problem to determine the minimum bandwidth (defined in USD) for each of the N classes that maximizes the revenue of the NAP, subject to satisfying a request blocking performance guarantee.

8. E.B. Dushanov, M. Emelianenko and G.Yu. Konovalova, *"On formats of the representation of real numbers and algorithm for automatic declaration of constants of the computer real arithmetic"*, J. Comput. Meth. Sci. Eng., **2**, issue 1-2 (2002), 57-62

Abstract. Formats of the representation for any-type numbers in different computers are presented. An algorithm for automatic definition of constants of the computer real arithmetic [1] is developed. Texts of programs on FORTRAN-77 realizing this algorithm as well as those extracting the exponent and mantissa of a real number are described.

## 2 In preparation

1. *"Toward a statistical theory for texture evolution"*, with Shlomo Ta'asan, David Kinderlehrer and Dmitry Golovaty, in preparation.

   Abstract. Recent years have witnessed a changing paradigm in experimental science: automated data acquisition technologies, now practiced in disciplines as varied as materials science and molecular biology, allow vast interrogation at certain scales. Typically most interesting are those mesoscales rich in information. The yield has been huge amounts of data being collected in many scientific disciplines, demanding novel approaches for interpretation. These advances pose new challenges for our understanding of such systems through mathematical modeling, simulation, and analysis.
   Our concern here is the mesoscopic behavior of the grain boundary system. One of the most challenging aspects is understanding the effect of critical events or topological reconfigurations during growth. In this paper, we study mesoscopic behavior of a one-dimensional grain boundary system and investigate the possibility of modeling texture evolution. One of the most challenging aspects of this problem is to understand the role of topological reconfigurations during coarsening. To this end, we investigate grain boundaries evolution in a "toy" one-dimensional system. We identify fractional nature of grain boundary kinetics and suggest a continuous time random walk framework that may be used to model this system in any dimension. We compare the predictions of the model with simulations and discuss its limitations and extensions to higher-dimensional cases.

2. *Boltzmann-type kinetic approach to grain growth dynamics*, with Shlomo Ta'asan, David Kinderlehrer and Dmitry Golovaty, in preparation.

   Abstract. We propose a new kinetic approach for describing mesoscopic behavior of a 1-dimensional grain boundary model. Depending on the level of dependencies one has the capacity to preserve, a set of nonlinear integro-differential equations is derived that captures system dynamics at longer or shorter periods of time. Connections with classical gas theory, advantages and limitations of the model as well as numerical illustrations are discussed. Due to a less restrictive nature of the molecular chaos assumption in higher dimensional cases, this model presents a high potential for practical applications.

3. *"Automation of High-dimensional Phase Diagram Calculation"*, with Zi-Kui Liu, in preparation.

   Abstract. This paper explores possible extensions of the previously presented method for automated phase diagram calculation to higher dimensions. Rigorous mathematical analysis of the sublattice models and the use of quasirandom sampling sequences form the basis for the construction and guarantee its cost-effectiveness.

4. *"Uniformly convergent two-dimensional nonlinear quantization scheme"*, with Ludmil Zikatanov, in preparation.

   Abstract. Numerical construction of optimal quantizers in two and three dimensional domains is the bottleneck of many practical problems. This paper generalizes previously presented 1-dimensional energy-based multilevel acceleration scheme to more general and complex domains by means of effective ordering and coarsening technques. Numerical examples are presented that demonstrate the advantages of the method in terms of complexity and time consumption for real applications.